

R & D facts

U.S. DEPARTMENT OF ENERGY
OFFICE OF FOSSIL ENERGY
NATIONAL ENERGY TECHNOLOGY LABORATORY

Chemistry and
Surface Science

3/2006



CONTACTS

Richard Noceti

Director
Chemistry and Surface Science
Division
National Energy Technology
Laboratory
626 Cochran's Mill Road
P.O. Box 10940
Pittsburgh, PA 15236-0940
412-386-5955
richard.noceti@netl.doe.gov

Bradley Bockrath

Physical Scientist
Chemistry and Surface Science
Division
National Energy Technology
Laboratory
626 Cochran's Mill Road
P.O. Box 10940
Pittsburgh, PA 15236-0940
412-386-6081
bradley.bockrath@netl.doe.gov

CUSTOMER SERVICE

I-800-553-7681

WEBSITE

www.netl.doe.gov



HYDROGEN MATERIALS LABORATORY

Full development of the hydrogen economy will require novel materials to enable effective separation and storage of this gas. Separation is important because a mixture of other gases is often generated along with the hydrogen. To satisfy the demands of Proton Exchange Membrane (PEM) fuel cells, undesirable components must be removed in a cost effective way. Storage systems that are compact, light weight, and conveniently charged and discharged must also be developed to meet the needs of practical fuel cell powered vehicles. New materials are continuously being developed to solve these problems.

The Hydrogen Materials Laboratory has the capacity to synthesize a wide variety of micro-porous materials suitable for storage and separation applications. Metal organic framework materials and porous metal salts are two examples. These materials retain hydrogen by simple physisorption. Charging and discharging is easy, rapid, and does not depend on heating or chemical reactions. The materials may be readily engineered to fit specific purposes by altering their pore dimensions or surface properties. They are used as powders for storage or pressure swing separation, or may be incorporated into porous membranes.

Adsorption isotherms, critical measures of adsorption strength and capacity, are measured over a wide range of pressure and temperature. A high resolution surface area instrument covers pressures up to one atmosphere, generally at liquid nitrogen or argon temperatures. A high pressure instrument covers pressures up to 100 atmospheres from liquid nitrogen to room temperature. Higher temperatures are available for special cases.

Direct observation of adsorbed gases is made with both infrared and Raman techniques. A specially constructed variable temperature, variable pressure, view cell obtains critical information on the specific sites responsible for adsorption. When gases are adsorbed, their infrared band is often shifted from that of free gas in a manner related to the nature of the sites it occupies. Further information on the relative binding strength of the sites is obtained from competition experiments by observing the displacement of one gas by another. The experimental results are compared with computer simulations to shed more light on the energetics of adsorption.